

REFERENCE POTENTIAL APPROACH TO THE QUANTUM-MECHANICAL INVERSE PROBLEM: II. SOLUTION OF KREIN EQUATION

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ABSTRACT. A reference potential approach to the one-dimensional quantum-mechanical inverse problem is developed. All spectral characteristics of the system, including its discrete energy spectrum, the full energy dependence of the phase shift, and the Jost function, are expected to be known. The technically most complicated task in ascertaining the potential, solution of a relevant integral equation, has been decomposed into two relatively independent problems. First, one uses Krein method to calculate an auxiliary potential with exactly the same spectral density as the initial reference potential, but with no bound states. Thereafter, using Gelfand-Levitan method, it is possible to introduce, one by one, all bound states, along with calculating another auxiliary potential of the same spectral density at each step. For the system under study (diatomic xenon molecule), the kernel of the Krein integral equation can be accurately ascertained with the help of solely analytic means. At small distances the calculated auxiliary potential with no bound states practically coincides with the initial reference potential, which is in full agreement with general theoretical considerations. Several possibilities of solving the Krein equation are proposed and the prospects of further research discussed.

1. INTRODUCTION

In this paper, a recently proposed reference potential approach to the one-dimensional quantum mechanical inverse problem [1] is further developed. Let us briefly recall that the starting idea is to choose a suitable reference potential for the system. For this fixed potential, it is always possible to calculate all its spectral characteristics, which means that in this artificial way one can obtain the complete set of information (otherwise inaccessible) needed to uniquely solve the inverse problem: 1) full energy spectrum of the bound states; 2) full energy dependence of the phase shift for the scattering states; 3) norming constants of the regular energy eigenfunctions for all bound states. Of course, there is no need to regain the potential which is already known by definition. However, the quantities related to the reference potential can be used as zeroth approximations to the real spectral characteristics of the system. A further step might be, for example, to calculate another potential whose discrete energy levels would exactly fit with their actually observed values, so that at least in this sense the new potential would be more realistic than the initial reference potential.

To illustrate the method, as previously, Xe_2 molecule is under study, and the same three-component exactly solvable reference potential is used. We have already ascertained the full energy dependence of the phase shift for the scattering states

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[1] and demonstrated its excellent agreement with the celebrated Levinson theorem [2]. In addition, we are provided with full knowledge of the Jost function, which is the most important spectral characteristic of the system. Thus, we are prepared to attack the most serious computational-technical problem, solution of an integral equation, which would enable to uniquely ascertain the potential. For this purpose a combined approach is used. In Section 2 we recall some useful properties of the Gelfand-Levitan method [3], which enable to separate the main problem into two independent parts: 1) calculating an auxiliary potential $V_0(r)$ with exactly the same spectral density for positive energies as the reference potential $V(r)$, but with no bound states; 2) calculating a series of auxiliary potentials $V_k(r)$, $k = 1, 2, \dots, n$ (i.e., adding, one by one, all bound states, and keeping their norming constants), also having the same spectral density for positive energies. The second step is, in fact, less complicated and is only briefly discussed in this paper. Our main goal is to ascertain the auxiliary potential $V_0(r)$ with no bound states, starting from the known Jost function for positive energies. This is the subject of Section 3 where the Krein method [4, 5] will be used. Some concluding remarks and a discussion of the further perspectives of the method form the content of Section 4.

2. STEP-BY-STEP USE OF GELFAND-LEVITAN METHOD

First, let us recall general solution scheme in the frame of Gelfand-Levitan method [3] (see, e.g., [6] for more details). One's aim is to solve the integral equation

$$(1) \quad K(r, r') + G(r, r') + \int_0^r K(r, s)G(s, r')ds = 0,$$

whose kernel

$$(2) \quad G(r, r') = \int_{-\infty}^{\infty} \frac{\sin(kr) \cdot \sin(kr')}{k^2} d\sigma,$$

is determined by the quantity $d\sigma \equiv \left[\frac{d\rho_2(E)}{dE} - \frac{d\rho_1(E)}{dE} \right] dE$, which contains the the difference of two spectral densities

$$(3) \quad \frac{d\rho(E)}{dE} = \begin{cases} \pi^{-1} \sqrt{E} |F(E)|^{-2}, & E \geq 0, \\ \sum_n C_n \delta(E - E_n), & E < 0, \end{cases}$$

one of them ($\frac{d\rho_1(E)}{dE}$) being related to a known potential ($V_1(r)$). In this sense Gelfand-Levitan method also represents a reference potential approach. The simplest possibility is to take $V_1(r) \equiv 0$, and correspondingly, $\frac{d\rho_1(E)}{dE} = \frac{\sqrt{E}}{\pi}$. Then

$$(4) \quad G(r, r') = \frac{2}{\pi} \int_0^{\infty} \sin(kr) \cdot \sin(kr') g(k) dk + \sum_n \frac{C_n}{4\gamma_n^2} \sinh(\gamma_n r) \sinh(\gamma_n r'),$$

where $\gamma_n^2 = -\frac{2mE_n}{\hbar^2}$, E_n being the bound levels and C_n , their related norming constants. The characteristic function

$$(5) \quad g(k) \equiv \frac{1}{|F(k)|^2} - 1$$

is determined by the modulus of the Jost function $F(k)$. Thus, in principle, one can solve Eq. (1) and then calculate the potential

$$(6) \quad V(r) = 2C \frac{d}{dr} K(r, r), \quad C \equiv \frac{\hbar^2}{2m}.$$

This scheme might seem simple, but its actual realization stumbles upon serious computational-technical difficulties. Now, let us assume that we somehow managed to ascertain an auxiliary potential $V_0(r)$ with exactly the same spectral density for positive energies as the desired potential $V(r)$, but having no bound states. In this case one easily finds that [6]

$$(7) \quad G(r, r') = \sum_j C_j \varphi_0(i\gamma_j, r) \varphi_0(i\gamma_j, r'),$$

where $\varphi_0(i\gamma_j, r)$ are the regular solutions (NB! not the real eigenfunctions!) related to the auxiliary potential $V_0(r)$. Next, let us introduce another auxiliary potential $V_1(r)$ with just one bound eigenvalue E_1 (note that numeration of the levels here starts from the highest-energy one, and therefore, E_n corresponds to the zeroth level), and again, with exactly the same spectral density for positive energies ($|F(k)|$ remains the same). Thereafter, one introduces an auxiliary potential $V_2(r)$ with two levels (E_1 and E_2), etc., until he comes to the desired potential $V_n(r) = V(r)$.

It can be proved that

$$(8) \quad V_j(r) - V_0(r) = -2C \{\ln [\det C_j(r)]\}'' , \quad j = 1, 2, \dots, n$$

and the corresponding regular solution

$$(9) \quad \varphi_j(k, r) = \det \begin{vmatrix} C_j(r) & \Psi_j(r) \\ \beta_j(k, r) & \varphi_0(k, r) \end{vmatrix} [\det C_j(r)]^{-1}.$$

Here, a $j \times j$ matrix $C_j(r) \equiv I + \int_0^r R^{(j)}(s) ds$ (I is the unit matrix) with the elements of $R^{(j)}$ being

$$(10) \quad R_{lm}^{(j)} = C_l \varphi_0(i\gamma_l, r) \varphi_0(i\gamma_m, r), \quad (l, m = 1, 2, \dots, j)$$

a column vector (do not confuse the norming constants C_l with the matrices $C_j(r)$)

$$(11) \quad \Psi_j(r) = \begin{pmatrix} C_1 \varphi_0(i\gamma_1, r) \\ C_2 \varphi_0(i\gamma_2, r) \\ \vdots \\ C_j \varphi_0(i\gamma_j, r) \end{pmatrix},$$

and a row vector

(12)

$$\beta_j(k, r) = \left(\int_0^r \varphi_0(i\gamma_1, s) \varphi_0(k, s) ds \int_0^r \varphi_0(i\gamma_2, s) \varphi_0(k, s) ds \dots \int_0^r \varphi_0(i\gamma_j, s) \varphi_0(k, s) ds \right)$$

have been introduced.

To be more specific, let us examine the simplest case of just one bound state ($j = 1$). Then $C_j(r)$ reduces to scalar and one gets

$$(13) \quad V_1(r) = V_0(r) - 2C \left\{ \ln \left[1 + C_1 \int_0^r \varphi_0^2(i\gamma_1, s) ds \right] \right\}''.$$

As can be shown [6], the regular solution $\varphi_1(i\gamma_1, r)$ related to $V_1(r)$ (i.e., the real confined eigenfunction) reads

$$(14) \quad \varphi_1(i\gamma_1, r) = \frac{\varphi_0(i\gamma_1, r)}{1 + C_1 \int_0^r \varphi_0^2(i\gamma_1, s) ds}.$$

Let us prove that C_1 , as needed, is the norming constant of $\varphi_1(i\gamma_1, r)$. Indeed, slightly rearranging Eq. (14): $1 + C_1 \int_0^r \varphi_0^2(i\gamma_1, s) ds = \frac{\varphi_0(i\gamma_1, r)}{\varphi_1(i\gamma_1, r)}$, differentiating both sides: $C_1 \varphi_0^2(i\gamma_1, r) = \frac{\varphi_0' \varphi_1 - \varphi_0 \varphi_1'}{\varphi_1^2}$, i.e., $C_1 \varphi_1^2(i\gamma_1, r) = -\left(\frac{1}{\varphi_0}\right)' \varphi_1 - \frac{1}{\varphi_0} \varphi_1' = -\left(\frac{\varphi_1}{\varphi_0}\right)'$, and integrating both sides of the latter equation, one gets $\int_0^\infty C_1 \varphi_1^2(i\gamma_1, r) dr = 1$, because any regular solution $\varphi(r) \approx r$ as $r \rightarrow 0$, and therefore, $\lim_{r \rightarrow 0} \left(\frac{\varphi_1}{\varphi_0}\right) = 1$.

Now, let us analyze a more complicated case of two bound states ($j = 1$). According to Eqs. (8) and (13),

(15)

$$V_2(r) - V_1(r) = V_2(r) - V_0(r) - [V_1(r) - V_0(r)] = -2C \left\{ \ln \left[\frac{\det C_2(r)}{1 + C_1 \int_0^r \varphi_0^2(i\gamma_1, s) ds} \right] \right\}''.$$

Here, the 2×2 matrix $C_2(r) = \begin{pmatrix} C_{11}(r) & C_{12}(r) \\ C_{21}(r) & C_{22}(r) \end{pmatrix}$ has the elements

$$(16) \quad C_{11}(r) = 1 + C_1 \int_0^r \varphi_0^2(i\gamma_1, s) ds, \quad C_{12}(r) = C_1 \int_0^r \varphi_0(i\gamma_1, s) \varphi_0(i\gamma_2, s) ds$$

$$C_{21}(r) = \frac{C_2}{C_1} C_{12}(r), \quad C_{22}(r) = 1 + C_2 \int_0^r \varphi_0^2(i\gamma_2, s) ds,$$

and therefore, the argument of the logarithm in Eq. (15) reads

$$(17) \quad f(r) \equiv C_{22} - \frac{C_1 C_2 \left[\int_0^r \varphi_0(i\gamma_1, s) \varphi_0(i\gamma_2, s) ds \right]^2}{1 + C_1 \int_0^r \varphi_0^2(i\gamma_1, s) ds} =$$

$$= 1 + C_2 \left\{ \int_0^r \varphi_0^2(i\gamma_2, s) ds - \frac{C_1 [\beta_{12}(r)]^2}{1 + C_1 \int_0^r \varphi_0^2(i\gamma_1, s) ds} \right\},$$

where $\beta_{12}(r) \equiv \int_0^r \varphi_0(i\gamma_1, s) \varphi_0(i\gamma_2, s) ds$.

As can be easily proved,

$$(18) \quad f(r) = 1 + C_2 \int_0^r \varphi_1^2(i\gamma_2, s) ds.$$

Indeed, using Eq. (14) and a more general formula [6]

$$\varphi_1(k, r) = \varphi_0(k, r) - C_1 \varphi_0(i\gamma_1, r) \times \frac{\int_0^r \varphi_0(i\gamma_1, s) \varphi_0(k, s) ds}{1 + C_1 \int_0^r \varphi_0^2(i\gamma_1, s) ds},$$

and taking $k = i\gamma_2$, one gets

$$\varphi_1(i\gamma_2, r) = \varphi_0(i\gamma_2, r) - C_1 \varphi_1(i\gamma_1, r) \beta_{12}(r),$$

i.e.,

$$\begin{aligned} \varphi_1^2(i\gamma_2, r) &= \varphi_0^2(i\gamma_2, r) + [C_1 \varphi_1(i\gamma_1, r) \beta_{12}(r)]^2 - 2C_1 \varphi_0(i\gamma_2, r) \varphi_1(i\gamma_1, r) \beta_{12}(r) = \\ &= \varphi_0^2(i\gamma_2, r) - C_1 \left[\frac{\varphi_1(i\gamma_1, r)}{\varphi_0(i\gamma_1, r)} \beta_{12}(r) \right]', \end{aligned}$$

which, after integrating from 0 to r , and taking account of Eq. (14), proves the claim.

Thus, in full analogy with Eq. (13), one can write

$$(19) \quad V_2(r) = V_1(r) - 2C \left\{ \ln \left[1 + C_2 \int_0^r \varphi_1^2(i\gamma_2, s) ds \right] \right\}'' ,$$

and more generally,

$$(20) \quad V_k(r) = V_{k-1}(r) - 2C \left\{ \ln \left[1 + C_k \int_0^r \varphi_{k-1}^2(i\gamma_k, s) ds \right] \right\}'' , \quad k = 1, 2, \dots, n.$$

This way one gets rid of inconvenient matrix equations and can move towards the goal step-by-step, introducing one bound state at a time.

The described procedure can be reverted [7, 8], i.e., starting from the potential $V_k(r)$, one can construct the auxiliary potential $V_{k-1}(r)$, removing the zeroth level

(E_k according to the numeration used). The new potential reads
(21)

$$V_{k-1}(r) = V_k(r) + 2C \left\{ \frac{2\Psi_0^{(k)}(r) \left(\Psi_0^{(k)}(r) \right)'}{\int_r^\infty \left(\Psi_0^{(k)}(s) \right)^2 ds} + \left[\frac{\left(\Psi_0^{(k)}(r) \right)^2}{\int_r^\infty \left(\Psi_0^{(k)}(s) \right)^2 ds} \right]^2 \right\}, \quad (k = n, n-1, \dots, 1)$$

where $\Psi_0^{(k)}(r)$ is the eigenfunction of the zeroth level, not necessarily normalized (note that the norming constant is absent here). One can remove, one by one, all bound states until he comes to the potential $V_0(r)$ with no bound states. An illustration to Eq. (21) can be seen in Fig. 1.

Thus, we have demonstrated that there is no need to solve Eq. (1) all at once. It is probably much easier to first solve this equation for the auxiliary potential $V_0(r)$ and then, step-by-step, introduce the bound states as described above. The Jost functions $F_n(k)$ and $F_0(k)$ related to the potentials $V_n(r)$ and $V_0(r)$, respectively, are connected by a simple formula

$$(22) \quad F_n(k) = F_0(k) \prod_{j=1}^n \left(\frac{k - i\gamma_j}{k + i\gamma_j} \right),$$

which demonstrates that these potentials, indeed, have exactly the same spectral densities for positive energies. On the other hand, Eq. (22) illustrates the general rule that any zero of the Jost function corresponds to a bound state.

To end this section, let us recall important asymptotic formulas (see [6] for details)

$$(23) \quad V_n(r) - V_0(r) \approx -4C \left(\sum_{j=1}^n C_j \right) r, \quad r \rightarrow 0,$$

$$(24) \quad V_n(r) - V_0(r) \approx -\frac{2C}{C_1} (2\gamma_1)^5 \exp(-2\gamma_1 r), \quad r \rightarrow \infty.$$

From Eq. (23) one can infer that in the immediate vicinity of the zero point $r = 0$ the potentials $V_n(r)$ and $V_0(r)$ practically coincide. Indeed, all norming constants $C_j = \left[\int_0^\infty \varphi_j^2(i\gamma_j, r) dr \right]^{-1}$ are extremely small quantities, since they are related to the regular solutions proportional to r as $r \rightarrow 0$, and vanishing as $r \rightarrow \infty$, but achieving very large absolute values between these asymptotic regions.

3. KREIN METHOD

Thus, in view of the results of previous section, our main goal is to accurately ascertain the auxiliary potential $V_0(r)$ with no bound states, provided that its spectral density $\frac{d\rho_0(E)}{dE} = \pi^{-1} \sqrt{E} |F(E)|^{-2}$ is known. This is indeed the case, since we have carefully calculated the modulus of the Jost function for the reference potential $V(r)$ [1], and the whole idea is to use the same quantity ($|F(E)|$) for the auxiliary potential $V_0(r)$ as well. Since there are no bound states, the kernel of the Gelfand-Levitan equation, according to Eq. (4), becomes analytically very simple:

$$(25) \quad G(r, r') = H(r - r') - H(r + r'),$$

where a new function

$$(26) \quad H(r) \equiv \pi^{-1} \int_0^{\infty} g(k) \cos(kr) dk,$$

with $g(k)$ given by Eq. (5), has been introduced. The function $H(r) = H(-r)$ is very important for the further treatment, wherefore a special designation, Krein H -function, will be used for this item henceforward. A motivation for this name stems from a very useful method for solving the inverse problem, which has been elaborated by Krein [4, 5]. This method is based on a Fredholm-type integral equation

$$(27) \quad \Gamma_{2r}(r') + H(r') + \int_0^{2r} \Gamma_{2r}(s) H(s - r') ds = 0.$$

It can be shown that the solutions of Gelfand-Levitan and Krein equations are linked by a simple formula (cf. with Eq. (25))

$$(28) \quad K(r, r') = \Gamma_{2r}(r - r') - \Gamma_{2r}(r + r'),$$

and the desired potential reads

$$(29) \quad V_0(r) = 4C \left\{ [G(x)]^2 - \frac{dG(x)}{dx} \right\}, \quad x \equiv 2r,$$

where $G(x) \equiv \Gamma_{2r}(2r)$. A special notation, Krein G -function, will be used for this quantity henceforward.

Without any doubt, Krein method is well suited for our purposes, but there is still a lot of analytical and computational-technical work to do. First, we have to accurately ascertain the Krein H -function, which, according to Eq. (26), is simply the Fourier cosine transform of the characteristic function $g(k)$ whose full energy dependence has already been ascertained [1]. One might think that the H -function can be determined using the well-known fast Fourier transform technique. This, however, is an erroneous view, because (as we demonstrate below) the H -function has to be calculated in a wide distance range with very small step, to ensure the correct asymptotic behavior of the resulting potential. Fortunately, the problem can be solved accurately and quite easily with the help of solely analytic means.

3.1. Calculation of H -function. The function $g(k)$ is shown in Fig. 2. In addition to the overall curve, some characteristic slices can be seen in the insets. There exists a range $k \in (0, k_1)$ where $g(k) = -1$ (with high accuracy), and for this range one immediately gets the relevant component of the H -function

$$H_0(r) = -\frac{\sin(k_1 r)}{\pi r}.$$

Now, let us see how the $g(k)$ curve passes through the "critical" region around $k_0 = \sqrt{V(0)/C}$. As it happens (see the upper inset in Fig. 2), in a narrow range $k \in (k_1, k_2)$ (k_0 is also located within this range) $g(k)+1$ can be nicely approximated by a sum of several Gaussians:

$$(30) \quad g(k) = -1 + \sum_j a_j \exp \left[-\frac{1}{2} \left(\frac{k - \tilde{k}_j}{b_j} \right)^2 \right],$$

where the parameters a_j, b_j and \tilde{k}_j can be determined from a least-squares fit. For the reference potential examined here, four such components have been introduced, and the value $k_2 = 19230 \text{ \AA}^{-1}$ has been chosen. Thus, in the above formula one can replace k_1 with k_2 (due to -1 in Eq. (30)), i.e.,

$$(31) \quad H_1(r) = -\frac{\sin(k_2 r)}{\pi r},$$

while the sum of Gaussians gives another component of the Krein H -function, $H_2(r) = \sum_j H_2^{(j)}(r)$, where all constituents $H_2^{(j)}(r)$ can be ascertained analytically.

Indeed, one can introduce a new independent variable $x \equiv \frac{k - \tilde{k}_j}{\sqrt{2}b_j}$, and calculate

$$(32) \quad H_2^{(j)}(r) = \frac{\sqrt{2}a_j b_j}{\pi} \int_{x_1}^{x_2} \exp(-x^2) \cos(\sqrt{2}b_j x r + \tilde{k}_j r) dx = \frac{a_j b_j}{\sqrt{2}\pi} \exp(-\frac{1}{2}b_j^2 r^2) \times \\ \times \left\{ \cos(\tilde{k}_j r) [\text{Re erf}(y_2) - \text{Re erf}(y_1)] - \sin(\tilde{k}_j r) [\text{Im erf}(y_2) - \text{Im erf}(y_1)] \right\},$$

where $x_l \equiv \frac{k_l - \tilde{k}_j}{\sqrt{2}b_j}$ and $y_l = x_l - \frac{ib_j r}{\sqrt{2}}$ ($l = 1, 2$ and i is the imaginary unit).

The error function, for any complex argument z , can be evaluated in terms of the confluent hypergeometric functions [9]

$$(33) \quad \text{erf}(z) = \frac{\sqrt{2}}{\pi} z \Phi\left(\frac{1}{2}, \frac{3}{2}; -z^2\right),$$

where $\Phi(a, c; x) = 1 + \frac{ax}{1!c} + \frac{a(a+1)x^2}{2!c(c+1)} + \dots$. For large arguments another expression is more convenient:

$$(34) \quad \text{erf}(z) = 1 - \frac{\exp(-z^2)}{\sqrt{\pi}z} \left[1 - \frac{1}{2z^2} + \frac{1 \cdot 3}{(2z^2)^2} - \frac{1 \cdot 3 \cdot 5}{(2z^2)^3} + \dots \right].$$

Consequently, any constituent of the Krein H -function expressed by Eq. (32) can be easily ascertained with any desired accuracy.

Next one can introduce an arbitrary (but still reasonable) boundary point k_3 , and approximate $g(k)$ in the range $k \in (k_2, k_3)$ as follows:

$$(35) \quad g(k) = \sum_j a_j \exp[-b_j(k - \tilde{k}_j)].$$

This brings along another component of the H -function $H_3(r) = \sum_j H_3^{(j)}(r)$ with constituents

$$(36) \quad H_3^{(j)}(r) = \frac{a_j}{\pi} \int_{k_2}^{k_3} \exp[-b_j(k - \tilde{k}_j)] \cos(kr) dk = \frac{a_j \exp(b_j \tilde{k}_j)}{\pi (b_j^2 + r^2)} \times \\ \times \{ \exp(-b_j k_3) [r \sin(k_3 r) - b_j \cos(k_3 r)] - \exp(-b_j k_2) [r \sin(k_2 r) - b_j \cos(k_2 r)] \}.$$

Introducing new suitable boundary points k_4, k_5 , etc., the approximation of $g(k)$ in the form of Eq. (35) can be continued until the conventional starting point k_a of

the asymptotic region (see the treatment below). The number of these boundary points, as well as the number of exponents in any particular interval, is, of course, a subject for probes and trials. We have introduced four such intervals and used a different three-exponent approximation in any of them. As has been carefully checked, this ensures the accuracy of at least 6 significant digits for the calculated Krein H -function in the whole physical domain. The parameters of all components are given in Table 1.

For the remaining part of the k -space the asymptotic formula

$$(37) \quad \ln |F(k)| = \frac{a_2}{k^2} + \frac{a_4}{k^4} + \frac{a_6}{k^6} + \dots, \quad k \geq k_a,$$

can be used, where [1]

$$(38) \quad a_2 = \frac{V(0)}{4C}, \quad a_4 = \frac{2[V(0)]^2 - CV''(0)}{16C^2}.$$

The coefficient a_6 , as well as the coefficients for higher-order terms, can also be calculated in terms of the reference potential and its derivatives, but the resulting expressions are rather complicated and inconvenient for practical use. Instead, we only introduced just one additional term, $\frac{a_6}{k^6}$, and determined the coefficient a_6 from the general demand (see Eq. (23)) that the potentials $V_0(r)$ and $V(r)$ should coincide as $r \rightarrow 0$. Such physically well motivated choice of a_6 is indeed possible, as will be explained below. Thus, within this approximation, the asymptotic part of $g(k)$ reads

$$(39) \quad g(k) = \frac{b_1}{k^2} + \frac{b_2}{k^4} + \frac{b_3}{k^6}, \quad k \geq k_a,$$

where

$$(40) \quad b_1 = -2a_2, \quad b_2 = -2(a_4 - a_2^2), \quad b_3 = -2(a_6 - 2a_2a_4 + \frac{2}{3}a_2^3).$$

The relevant asymptotic component of the H -function becomes

$$H_a(r) \equiv \pi^{-1} \int_{k_a}^{\infty} g(k) \cos(kr) dk.$$

Since the expression for $H_a(r)$ will contain the sine integral $\text{Si}(x_a) \equiv \int_0^{x_a} \frac{\sin t}{t} dt$, let us recall a useful formula [9]

$$(41) \quad \text{Si}(x) = \frac{\pi}{2} - \frac{i}{2} \exp(-ix) \Psi(1, 1; ix) + \frac{i}{2} \exp(ix) \Psi(1, 1; -ix),$$

where i is the imaginary unit, and the function $\Psi(a, c; z)$ is a particular solution of the confluent hypergeometric equation introduced by Tricomi. For a large argument it can be evaluated from the asymptotic series

$$(42) \quad \Psi(a, c; z) = z^{-a} \sum_{n=0}^N \frac{(a)_n (a - c + 1)_n}{n! (-z)^n},$$

where $(a)_n \equiv \Gamma(a + n)/\Gamma(a) = a(a + 1)(a + 2) \dots (a + n - 1)$ is the Pochhammer symbol, and N must not be too large. If Eq. (41) is usable, i.e., in the case of

sufficiently large r , one gets the following expression:

$$(43) \quad \pi H_a(r) = \left(\frac{b_1 A_1}{1! k_a} - \frac{b_2 A_2}{3! k_a^3} + \frac{b_3 A_3}{5! k_a^5} \right) \frac{\sin(x_a)}{x_a} - \left(\frac{b_1 B_1}{1! k_a} - \frac{b_2 B_2}{3! k_a^3} + \frac{b_3 B_3}{5! k_a^5} \right) \frac{\cos(x_a)}{x_a^2}, \quad x_a \equiv k_a r \gg 1,$$

where

$$A_i = \sum_{j=0}^{\infty} \frac{(-1)^{i+j} [2(i+j)-1]!}{(x_a)^{2j}}, \quad B_i = \sum_{j=0}^{\infty} \frac{(-1)^{i+j} [2(i+j)]!}{(x_a)^{2j}}, \quad i = 1, 2, 3.$$

If Eq. (41) cannot be used, one can apply the universal expansion

$$(44) \quad \text{Si}(x_a) = x_a - \frac{(x_a)^3}{3 \cdot 3!} + \frac{(x_a)^5}{5 \cdot 5!} - \dots,$$

to get another formula

$$(45) \quad \pi H_a(r) = \left(\frac{b_1 r}{1!} - \frac{b_2 r^3}{3!} + \frac{b_3 r^5}{5!} \right) \left[\text{Si}(x_a) - \frac{\pi}{2} \right] + \left(\frac{b_1 X_0}{1! k_a} - \frac{b_2 X_1}{3! k_a^3} + \frac{b_3 X_2}{5! k_a^5} \right) \cos(x_a) - r \left(\frac{b_2 Y_0}{3! k_a^2} - \frac{b_3 Y_1}{5! k_a^4} \right) \sin(x_a),$$

$$(46) \quad X_i = \sum_{j=0}^i (-1)^{i-j} [2(i-j)]! (x_a)^{2j}, \quad Y_i = \sum_{j=0}^i (-1)^{i-j} [2(i-j)+1]! (x_a)^{2j}.$$

From Eq. (45) one can infer that near the zero point $r = 0$

$$H_a(r) \approx \pi^{-1} \left(\frac{b_1}{k_a} + \frac{b_2}{3k_a^3} + \frac{b_3}{5k_a^5} \right) - \frac{b_1 r}{2},$$

and consequently, according to Eqs. (38) and (40), the derivative at zero point $[H_a(0)]' = -\frac{b_1}{2} = \frac{V(0)}{4C}$. Let us prove that the same relation holds for the overall Krein H -function. Indeed, as $r \rightarrow 0$, one can always choose a value for k_a which is large enough, so that Eq. (39) can be used, but on the other hand, small enough, so that $\sin(kr) \approx kr$, if $k \in (0, k_a]$. Integrating by parts (note that $g(\infty) = 0$), one gets from Eq. (26)

$$\pi H(r \rightarrow 0) = - \int_0^{k_a} g'(k) k dk + \frac{2}{r} \int_{k_a}^{\infty} \left(\frac{b_1}{k^3} + \frac{2b_2}{k^5} + \frac{3b_3}{k^7} + \dots \right) \sin(kr) dk.$$

Only the second term gives contribution to $H'(0)$, and after few elementary transformations one comes to the desired result

$$(47) \quad H(r \rightarrow 0) = -\frac{b_1 r}{2} + \pi^{-1} \int_0^{\infty} g(k) dk,$$

which proves that

$$(48) \quad H'(0) = -\frac{b_1}{2} = \frac{V(0)}{4C}.$$

Thus, in the case examined here, the Krein H -function can be, indeed, ascertained analytically. To get the overall H -function, one just sums the components

described above: $H(r) = \sum_j H_j(r)$. The result for different distance regions is shown in Figs. 3 and 4. As can be seen, $H(r)$ is a rapidly oscillating function with decaying amplitude. The period of oscillations stabilizes quite rapidly and remains very close to the characteristic value $L = \frac{2\pi}{k_2}$ (see Eq. (31)), while the amplitude slowly approaches zero as $r \rightarrow \infty$.

3.2. Solution of Krein equation. Before setting about the main task, we have to fix the coefficient b_3 in Eq. (39). To this end, let us take into consideration that according to Eq. (27), $G(0) = -H(0)$. Also, as repeatedly mentioned (see Eq. (23)), the potentials $V_0(r)$ and $V(r)$ should coincide as $r \rightarrow 0$. One therefore can replace $V_0(r)$ with $V(r)$ in Eq. (29), when studying the region very close to $r = 0$. In addition, the Krein G -function there can be approximated by a quadratic function: $G(x) = a + bx + cx^2$ ($x = 2r$), and consequently, $G'(x) = b + 2cx$. In this region a pseudo-Morse approximation for the reference potential is used: $V(r) = V_0 + A_0 \exp(-\alpha_0 x) - \sqrt{A_0 \varepsilon_0} \exp(-\alpha_0 x/2)$. Here, $A_0 \equiv D_0 \exp(2\alpha_0 r_0)$ and $\varepsilon_0 \equiv D_0/4$ (see [1] for more details). Therefore, the parameters a, b, c can be ascertained directly from Eq. (29). Indeed, one uses the relations $N_1 \equiv a^2 - b = \frac{V(0)}{4C}$, $N_2 \equiv c - ab = \frac{\alpha_0(A_0 - \sqrt{A_0 \varepsilon_0}/2)}{8C}$, $N_3 \equiv b^2 + 2ac = \frac{\alpha_0^2(4A_0 - \sqrt{A_0 \varepsilon_0})}{32C}$, then solves the equation $(a^2 - N_1)^2 + 2a[a(a^2 - N_1) + N_2] - N_3 = 0$ to ascertain the parameter $a = G(0) = -H(0)$, and thereafter finds b and c . Having fixed these parameters, and also the value of k_a , the coefficient b_3 can be quite easily determined on a trial-by-trial basis. This way the value $b_3 = -5.883044 \cdot 10^{24} \text{ (\AA}^{-6}\text{)}$ has been fixed, which corresponds to $k_a = 75000 \text{ \AA}^{-1}$.

Now, let us proceed with solution of Eq. (27). This equation can be discretized using, for example, a four-point quadrature rule [10]

$$(49) \quad \int_{kh}^{(k+3)h} f(x)dx = \frac{3h}{8}f(kh) + \frac{9h}{8}f([k+1]h) + \frac{9h}{8}f([k+2]h) + \frac{3h}{8}f([k+3]h),$$

which is exact for $f(x)$ a cubic polynomial. Applying this formula to Eq. (27), one gets the following system of linear equations:

$$(50) \quad (1 + \Delta H_0) \Gamma_{3n,0} + 3(\Delta H_1 \Gamma_{3n,1} + \Delta H_2 \Gamma_{3n,2}) + 2\Delta H_3 \Gamma_{3n,3} + \\ + 3(\Delta H_4 \Gamma_{3n,4} + \Delta H_5 \Gamma_{3n,5}) + 2\Delta H_6 \Gamma_{3n,6} + \dots + \Delta H_{3n} \Gamma_{3n,3n} = -H_0$$

$$\Delta H_{-1} \Gamma_{3n,0} + (1 + 3\Delta H_0) \Gamma_{3n,1} + 3\Delta H_1 \Gamma_{3n,2} + 2\Delta H_2 \Gamma_{3n,3} + \dots + \Delta H_{3n-1} \Gamma_{3n,3n} = -H_1$$

$$\Delta H_{-2} \Gamma_{3n,0} + 3\Delta H_{-1} \Gamma_{3n,1} + (1 + 3\Delta H_0) \Gamma_{3n,2} + \dots = -H_2$$

$$\Delta H_{-3} \Gamma_{3n,0} + 3(\Delta H_{-2} \Gamma_{3n,1} + \Delta H_{-1} \Gamma_{3n,2}) + (1 + 2\Delta H_0) \Gamma_{3n,3} + \dots = -H_3$$

$$\vdots$$

$$\Delta H_{-3n} \Gamma_{3n,0} + 3(\Delta H_{1-3n} \Gamma_{3n,1} + \Delta H_{2-3n} \Gamma_{3n,2}) + (1 + \Delta H_0) \Gamma_{3n,3n} + \dots = -H_{3n}$$

or, in a more compact form,

$$(51) \quad \Gamma_{3n,k} + \Delta \cdot (H_{-k}\Gamma_{3n,0} + 3H_{1-k}\Gamma_{3n,1} + 3H_{2-k}\Gamma_{3n,2} + 2H_{3-k}\Gamma_{3n,3} + \dots + H_{3n-k}\Gamma_{3n,3n}) = -H_k, \quad k = 0, 1, 2, \dots, 3n.$$

Here $\Delta \equiv \frac{3h}{8}$, $H_k = H_{-k} = H(kh)$, and $\Gamma_{3n,k} \equiv \Gamma_{2r}(kh)$ (see Eq. (27)).

For any argument $x = 2r = 3nh$, Eq. (50) can be solved with the help of Gaussian elimination procedure, which is appropriate here, since only the last element of the solution vector, $\Gamma_{3n,3n} = \Gamma_{2r}(2r) = G(x)$ is actually needed to calculate the potential according to Eq. (29). Alternatively, one may rewrite Eq. (51) in a matrix form

$$(52) \quad (I + \Delta \cdot U) \cdot G = -H,$$

where I denotes $(3n+1) \times (3n+1)$ unit matrix,

$$G \equiv \begin{pmatrix} \Gamma_{3n,0} \\ \Gamma_{3n,1} \\ \vdots \\ \Gamma_{3n,3n} \end{pmatrix}, \quad H \equiv \begin{pmatrix} H_0 \\ H_1 \\ \vdots \\ H_{3n} \end{pmatrix},$$

and

$$U \equiv \begin{pmatrix} H_0 & 3H_1 & 3H_2 & 2H_3 & \dots & 3H_{3n-1} & H_{3n} \\ H_1 & 3H_0 & 3H_1 & 2H_2 & \dots & 3H_{3n-2} & H_{3n-1} \\ & & & \vdots & & & \\ & & & & & & \\ H_{3n} & 3H_{3n-1} & 3H_{3n-2} & 2H_{3n-3} & \dots & 3H_1 & H_0 \end{pmatrix}.$$

The solution of Eq. (52) reads

$$(53) \quad G = -(I + \Delta \cdot U)^{-1} \cdot H = -H + \Delta \cdot U \cdot H - \Delta^2 \cdot U^2 \cdot H + \dots,$$

and therefore,

$$(54)$$

$$\Gamma_{3n,3n} = -H_{3n} + \Delta \cdot (H_{3n}H_0 + 3H_{3n-1}H_1 + 3H_{3n-2}H_2 + 2H_{3n-3}H_3 + \dots + H_0H_{3n}) - \Delta^2 \cdot \sum_{i,j} g_i g_j H_{3n-i} H_{|i-j|} H_j + \dots$$

The coefficients g_i (here and henceforward) are defined as follows: $g_i = 1$, if $i = 0$ or $i = m \equiv 3n$; $g_i = 2$, if $i = 3k$ and $k = 1, 2, \dots, n-1$; $g_i = 3$ in any other case.

According to Eqs. (6) and (28), $V(r) = 4C \left\{ \frac{d\Gamma_x(0)}{dx} - \frac{d\Gamma_x(x)}{dx} \right\}$. Comparing this with Eq. (29), one gets an important relation

$$(55) \quad \frac{d\Gamma_x(0)}{dx} = [G(x)]^2, \quad (x = 2r)$$

Thus, instead of searching for the last element of the solution vector G , one may calculate its first element Γ_{m0} ($m = 3n$), which in some sense is more convenient.

Indeed, using such an approach, we can make use of the results of previous calculations. Namely, as can be proved

$$(56) \quad \Gamma_{m+3,0} = \Gamma_{m0} + \Delta \cdot (H_m^2 + 3H_{m+1}^2 + 3H_{m+2}^2 + H_{m+3}^2) - \Delta^2 \cdot S_m + \dots$$

where

$$(57)$$

$$S_m = 2 \sum_{j=0}^{m-1} g_j H_j (H_m H_{m-j} + 3H_{m+1} H_{m+1-j} + 3H_{m+2} H_{m+2-j} + H_{m+3} H_{m+3-j}) + \\ H_0 (3H_m^2 + 9H_{m+1}^2 + 9H_{m+2}^2 + H_{m+3}^2) + 6H_1 (H_{m+3} H_{m+2} + 3H_{m+2} H_{m+1} + 2H_{m+1} H_m) + \\ + 6H_2 (H_{m+3} H_{m+1} + 2H_{m+2} H_m) + 4H_3 H_{m+3} H_m, \quad m = 0, 1, 2, \dots$$

From Eqs. (55) and (56) one gets another formula

$$(58) \quad 8[G(x)]^2 = H_m^2 + 3H_{m+1}^2 + 3H_{m+2}^2 + H_{m+3}^2 - \Delta \cdot S_m + \dots, \quad x = mh,$$

which may prove very useful, if the higher order terms can be ignored.

In Fig. 5 one can see the calculated Krein G -function in the range from 0 to 10^{-6} Å. Eq. (50) has been solved by Gaussian elimination, and an extremely small step $h = 10^{-9}$ was used to ensure high accuracy. For comparison, another curve (actually, almost straight line) is depicted, which exactly corresponds to the reference potential $V(r)$, i.e., it is the solution of Eq. (29) interpreted as Riccati equation:

$$(59) \quad \frac{dG(x)}{dx} = [G(x)]^2 - \frac{V(x/2)}{4C}, \quad G(0) = -H(0).$$

The curves practically coincide, which is a clear evidence of the validity of the approach. Indeed, this seemingly trivial calculation is, in fact, very sensitive to even minor inaccuracies in calculating the Krein H -function, which would result in undesired and unphysical discrepancies, e.g., oscillations, of the G -function. Since no such discrepancies are seen at small distances, one may expect that both the Jost function and the H -function have been ascertained quite correctly. This in turn gives ground to hope that the potential can be correctly ascertained at longer distances as well. This, however, is not at all an easy task, and was not attempted here.

4. CONCLUSION

In this paper, as well as in the previous one [1], the treatment was more concentrated on principles rather than the methods and techniques of computation. We demonstrated that the proposed reference potential approach enables one to accurately ascertain the important spectral characteristics, needed to uniquely solve the quantum-mechanical inverse problem. This way, one may get reasonable initial guesses to the real spectral characteristics of the system, which can be used, for example, to calculate another potential (Bargmann potential) whose Jost function differs from the initial one only by a rational factor. Let us briefly analyze the simplest case when this factor reads

$$(60) \quad \frac{k - ia}{k + ib} = \frac{k - ia}{k + ia} \cdot \frac{k + ia}{k + ib},$$

where both, a and b , are real and positive. In fact, it means that a discrete eigenvalue $-b^2$ is replaced by $-a^2$. As we see, Eq. (60) involves two operations. One of

them, introducing a new bound state $E = -a^2$, can be performed as described in Section 2, while the second factor, $\frac{k+ia}{k+ib}$, causes an additional deformation of the initial potential [6]

$$(61) \quad \Delta V(r) \equiv V_2(r) - V_1(r) = -2C \left\{ \ln \frac{W[f_1(ia, r), \varphi_1(ib, r)]}{b^2 - a^2} \right\}'' ,$$

where the symbol W denotes Wronskian determinant and $f_1(ia, r)$ is the Jost solution of the Schrödinger equation ($f_1(ia, r) \rightarrow \exp(-ar)$ as $r \rightarrow \infty$). Both $f_1(ia, r)$ and the regular solution $\varphi_1(ib, r)$ are related to the potential $V_1(r)$. Thus, if $-a^2$ is expected to be more realistic eigenvalue than $-b^2$, one may hope that $V_2(r)$ is more realistic potential than $V_1(r)$ as well.

The proposed approach is based on various analytic procedures. For example, we used piecewise analytic approximation for the characteristic function $g(k)$ (see Eq. (5) and Fig. 2), and derived simple formulas for relevant constituents of the Krein H -function. In addition, we proved some general relations, Eqs. (47) and (48), regarding H -function near the zero point $r = 0$, and fixed an appropriate value for $G(0) = -H(0) = \pi^{-1} \int_0^\infty g(k)dk$ (see Section 3.2), which ensures the correct behavior of the resulting potential in this region.

One of our goals was to promote Krein method [4, 5] to solve the inverse problem. This method is especially suitable to ascertain the auxiliary potential $V_0(r)$ with no bound states, starting from the known Jost function. Having ascertained $V_0(r)$, one can build up a series of auxiliary potentials: $V_1(r)$, $V_2(r)$, ..., $V_n(r)$, introducing, one by one, all bound states with known eigenvalues. Several possibilities of solving the main integral equation, Eq. (27), have been proposed and discussed, but not yet fully exploited. From the computational-technical point of view the problem is much more complicated than it might seem at first sight. Indeed, to ascertain, for example, the correct position of the most right-side point in Fig. 5, a system of 999 equations has been solved. One can imagine that it is not so easy to extend calculations to much larger distances than shown in Fig. 5. Perhaps, to bridge over these technical difficulties, one can take some advantage of Eqs. (54) and (56), which seem to be straightforward and useful solution schemes. On the other hand, rapid development of parallel computing and Grid technology, as well as prospects of quantum computing, also suggest some optimism for further research in this field.

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FIGURE CAPTIONS

- Fig. 1. Abraham-Moses [7] trick applied to three-component model potential for Xe_2 (in ground electronic state). Each step consists of removing the zeroth level along with calculating the new potential according to Eq. (21). The depth of the potential well is about 24.3 meV and the original reference potential (curve 1) has 24 levels. Although only 5 lowest partner potentials (all having the same spectral density for positive energies) are shown, they roughly demonstrate that all partner potentials should coincide as $r \rightarrow 0$. In addition, the presented curves might help to imagine how the auxiliary potential with no bound states would look like.
- Fig. 2. Demonstration of the characteristic function $g(k)$ given by Eq. (5). The overall $g(k)$ curve shown in the main figure seems to decay rapidly, but this impression is deceptive, because the k scale is logarithmic. As can be seen, $g(k) = -1$ (with high accuracy), if $k \lesssim k_0 = \sqrt{V(0)/C}$. The insets demonstrate how nicely the different intervals can be described by a sum of Gaussians (upper inset) or exponents (lower inset) according to Eqs. (30) and (35), respectively. Parameters of the different components are given in Table 1, and Eq. (39) has been used for the region $k \geq k_a = 75000 \text{ \AA}$.
- Fig. 3. Calculated Krein H -function in the immediate vicinity of the zero point $r = 0$.
- Fig. 4. Another demonstration of the Krein H -function. The upper graph starts where Fig. 3 ends, while the lower graph starts where the upper one ends. Note that the period of oscillations is nearly constant and very close to the characteristic value $L = \frac{2\pi}{k_2}$ (see Eq. (31)).
- Fig. 5. Calculated G -function as a solution of Eq. (50) (solid curve), i.e., corresponding to the auxiliary potential $V_0(r)$ with no bound states. Note that the G -curve falls much slower than the H -curve ascends (cf. with Fig. 3). Another curve (open circles) has been calculated according to Eq. (59), and is therefore directly related to the reference potential $V(r)$. Since these differently calculated curves practically coincide, the two potentials in question also coincide in the range depicted.

TABLE 1. Fitting parameters for the characteristic function $g(k)$ defined by Eq. (5). In all cases k_a denotes the starting point of the distance range, while k_b marks its end point.

$k_a(1/\text{\AA})$	$k_b(1/\text{\AA})$	j	a_j (dimensionless)	b_j	$\tilde{k}_j(1/\text{\AA})$
0	19230	1	0.0642222322635	28.571730018198	19266.4518
based on	Eq. (30)	2	0.0427640496056	31.693733469307	19214.4537
b_j unit:	$1/\text{\AA}$	3	$1.313714415*10^{-3}$	18.093176481161	19169.6355
		4	$-2.18368077*10^{-5}$	8.5288122450848	19153.495
19230	20000	1	0.0221286191169	0.0130759575537	19230
based on	Eq. (35)	2	0.1065231936499	0.0024849989851	19230
b_j unit:	\AA	3	0.8049658419302	$1.764449543*10^{-4}$	19230
20000	21890	1	$6.56300549*10^{-3}$	0.0028620459089	20000
based on	Eq. (35)	2	0.1165529570422	$7.050434325*10^{-4}$	20000
b_j unit:	\AA	3	0.5953096962391	$1.049812095*10^{-4}$	20000
21890	43600	1	0.0384392174818	$5.707750043*10^{-4}$	21890
based on	Eq. (35)	2	0.2498847654991	$1.654292141*10^{-4}$	21890
b_j unit:	\AA	3	0.2306247842633	$4.074037076*10^{-5}$	21890
43600	75000	1	0.0113479356044	$1.341135741*10^{-4}$	43600
based on	Eq. (35)	2	0.0540153535949	$5.355103398*10^{-5}$	43600
b_j unit:	\AA	3	0.0367554032472	$1.488005999*10^{-5}$	43600
75000	∞	1		184142158.24434	(\AA^{-2})
based on	Eq. (39)	2		$1695416626*10^{16}$	(\AA^{-4})
		3		$-5.883044*10^{24}$	(\AA^{-6})

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